



Growth direction selection of tilted dendritic arrays in directional solidification over a wide range of pulling velocity: A phase-field study



Hui Xing^{a,*}, Kumar Ankit^b, Xianglei Dong^a, Huimin Chen^a, Kexin Jin^a

^aThe Key Laboratory of Space Applied Physics and Chemistry, Northwestern Polytechnical University, 710129 Xi'an, PR China

^bMaterials Science and Engineering, School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ 85287, United States

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ABSTRACT

In this paper, the growth direction selection of tilted dendritic arrays in directional solidification over a wide range of pulling velocity was investigated by using a thin-interface phase-field model. A systematic convergence study with respect to the interface width for various pulling velocities was first carried out to keep simulated results that are independent of interface width. In our simulations, all data points effectively collapse to the DGP (Deschamps, Georgelin, and Pocheau) law (Phys Rev E **78** (2008) 011605-1-13) for lower pulling velocities while numerical results departure from the DGP law for higher pulling velocity. Based on the data from phase-field simulations, we discussed the dependence of the coefficients f and g in DGP law on μ ($\mu = V_p/V_c$) for a fixed misorientation angle. The dendritic tip shapes of tilted and non-tilted dendrites were compared, and the evolution of tip radius with the variation of V_p was studied. Then, we discuss the reason why our numerical results departure from the DGP law for larger pulling velocities based on the variation of dendritic tip radius with the increase of the pulling velocity for a given Péclet number.

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1. Introduction

In directional solidification, the melt is forced to solidify at a constant pulling velocity V_p through a fixed temperature gradient G [1]. Once the constitutional undercooling ahead of the solidifying front overcomes the interface-stabilizing thermal gradient, the dendritic structures originating from the well-known Mullins-Sekerka instability [2] arise at the solid-liquid interface when the pulling velocity is above a critical pulling speed. Since the dendritic structures have a strong influence on the mechanical properties of the solidified casting, understanding of its growth dynamics is of major scientific and technological interests [1]. The characterization of the preferred crystallographic direction is one of the most important aspects of the growth of the dendritic arrays. There are two specific directions having influence on the growth and evolution of dendritic arrays: the thermal gradient direction and the preferred crystallographic direction. When the two directions differ, the competition between them determines the real growth direction of the dendritic arrays as well as interfacial morphologies.

Experiment conducted in thin samples of transparent organic alloys is a particularly suitable tool to study the growth direction selection of dendritic arrays due to the allowable direct observation of the interfacial morphological evolution by an optical microscopy [3]. Previous experimental investigations [4–9] show that the real growth direction of dendritic arrays undergoes a continuous variation from the thermal gradient direction to the preferred crystalline orientation as well as the dramatic changes of interfacial morphologies with the increase of the pulling velocity. In thin sample experiments of directional solidification of $\text{CBr}_4\text{-C}_2\text{Cl}_6$, Akamatsu and Ihle [6] firstly found that the real growth direction depends on the Péclet number ($Pe = V_p\Lambda/D_l$, where Λ is primary spacing, V_p pulling velocity, and D_l the solute diffusivity in the liquid). However, a quantitative relationship between the real growth direction and the Péclet number is not given. Through carrying out systematic thin sample experiments of directional solidification of a succinonitrile-ethylene alloy over a range of pulling velocity, Deschamps et al. [9] correlated the real growth direction angle Θ (the angle between the growth direction of dendritic arrays and the thermal gradient direction) to both the misorientation angle Θ_0 and the Péclet number Pe ($Pe = V_G\Lambda/D_l$, where V_G is the pulling velocity projected on the thermal gradient direction) according to the DGP law,

* Corresponding author.

E-mail addresses: huixing@nwpu.edu.cn (H. Xing), kumar.ankit@tamu.edu (K. Ankit).

$$\Theta = \Theta_0 - \Theta_0 [1 + f(\Theta_0) Pe^g]^{-1}, \quad (1)$$

with

$$f(\Theta_0) = \alpha \left[1 - (\Theta_0 / \Theta_m)^\beta \right], \quad (2)$$

with $\alpha = 1.1$, $\beta = 4$, $\Theta_m = 46^\circ$ and $g = 1.25$. This law indicates that the real growth direction angle Θ versus the Péclet number Pe yields a common non-linear function, i.e., $\Theta \rightarrow 0$ for $Pe \rightarrow 0$ and $\Theta \rightarrow \Theta_0$ for a relatively large Pe . Hence, the DGP law describes the continuous variation of dendritic growth direction from the thermal gradient direction to the preferred crystalline orientation observed in experiments. Experimental results by Akamatsu and Ihle [6] show that values of the coefficients f and g are $f(34.5^\circ) \approx 0.64$, $f(43.6^\circ) \approx 0.47$ and $g \approx 1.6$ for $\text{CBr}_4\text{-C}_2\text{Cl}_6$, which are comparable to the results by Deschamps et al. [7–9]. With the help of the development of the numerical methods, the growth direction selection of dendritic arrays has been investigated in two- and three-dimensional systems [6,10–14]. Although Ghmadh et al. [12] found that three-dimensional simulations are necessary for obtaining accurate quantitative predications by comparing experimental results and phase-field simulations, it was shown that a good agreement with experiments can be also provided by two-dimensional simulations. Two-dimensional phase-field simulations for a wide range of misorientation angles by Tournet and Karma [14] show that the dendritic growth direction can be modeled by the DGP law with different values of the coefficients f and g .

However, we cannot avoid the limitation of the DGP law. Firstly, the effect of the surface tension anisotropy (properties of materials) on the growth direction selection is not involved in the DGP law; secondly, whether the coefficients f and g vary over a wider range of pulling velocity is still unclear. Previous numerical work show that the coefficients f and g depend sensitively on the alloy parameters [6,13]. Two-dimensional phase-field simulations offer $f(30^\circ) \approx 0.76$ and $g \approx 1.47$ for a Ni-based alloy [11] and $f(30^\circ) \approx 0.2$ and $g \approx 1.925$ for an Al-based alloy [13] at relatively large pulling velocities. In our previous work [15], the dependence of f and g in the DGP law on ε_4 was systematically investigated for a wide range of Θ_0 to extend the DGP law, showing that both coefficients f and g indeed can be expressed as a nonlinear function of ε_4 . Furthermore, for a wider range of pulling velocity, it was found that f decreases and g increases with the decrease of pulling velocity. Indeed, this finding challenges the factor that the growth direction solely depends on the Péclet number. Therefore, while the growth direction selection of dendritic arrays is not a very novel topic, the quantitative description of the growth direction selection for a wide range of pulling velocity is more complex than what we previously expected. Motivated by our previous finding, we shed light on the growth direction selection of dendritic arrays in directional solidification over a wide range of pulling velocity through two-dimensional phase-field simulations. The remainder of this paper is organized as follows: firstly, we briefly describe the thin-interface phase-field model, and a convergence study with respect to the coupling constant λ for various pulling velocities is carried out in Section 2. In Section 3, we present our numerical results. A discussion of the results is given in Section 3. The conclusions of this study are presented in Section 4.

2. Model descriptions and convergence study

We use the thin-interface phase-field model of dilute-alloy directional solidification by Karma [16] and Echebarria et al. [17] to investigate tilted growth of dendritic arrays over a wide range of pulling velocity. In this model, the added anti-trapping term recovers local equilibrium at the interface and eliminates spurious effects due to the diffuse interface. Detailed derivation of this

model can be found in the Ref. [17]. For simplicity, we neglect the diffusion in the solid. Since the latent heat production is neglected, for convenience, the so-called “frozen temperature approximation” is used here for the directional solidification, $T = T_{ref} + G(z - V_p t)$, where T_{ref} is a reference temperature. Our phase-field simulations will be compared with the experimental work by Deschamps et al. [9]. In their experiments, the object is a nearly pure but actually not pure transparent plastic crystal, the succinonitrile. An NMR study reveals that the dominant impurity involves an ethylenic chemical bond. Therefore, the impure alloy can be considered as a very dilute alloy. In experiments, it is very difficult to determine the real impurity concentration. However, systematic experimental studies can provide: solute partition coefficient k and mc_0 , where m is the liquidus slope, c_0 is the solutal concentration [3]. Therefore, in our simulations, solute partition coefficient $k = 0.29$, the product of the liquidus slope and solutal concentration $|m|c_0 = 2.0$ K, liquid diffusion coefficient $D_l = 1350 \mu\text{m}^2/\text{s}$, Gibbs–Thomson coefficient $\Gamma = 0.0648 \text{ K}\cdot\mu\text{m}$ in order to quantitatively compare our results with the DGP law [9]. The pulling velocity V_p is in the range from $15 \mu\text{m}/\text{s}$ to $300 \mu\text{m}/\text{s}$, and the thermal gradient G is fixed at $0.014 \text{ K}/\mu\text{m}$ unless otherwise noted. In the constitutional undercooling approximation, the cellular-threshold velocity V_c is calculated through $V_c = D_l G / |m|(1/k - 1)$. These solidification conditions put the system in dendritic regime. For tilted dendrites, the misorientation angle is fixed at $\Theta_0 = 30^\circ$ since larger misorientation angle may lead to seaweed patterns [18]. The contribution of the misorientation angle has been shown in Eq. (2). For impure succinonitrile (SCN) alloy system, the anisotropy of the interfacial free energy $\varepsilon_4 = 0.007$ (0.7%) is generally used in phase-field simulations (e.g. [12,19]).

Fig. 1 schematically shows the growth of tilted dendritic arrays in directional solidification, where \mathbf{a} presents the preferred crystalline direction, \mathbf{G} is the thermal gradient, \mathbf{V}_g the real growth velocity whose direction is between the preferred crystallographic direction and the thermal gradient direction, Θ_0 the misorientation angle, Θ the real growth direction angle, Λ the spacing between two dendrites. In this phase-field model, τ_0 and W_0 are the time and length scales, respectively. To avoid kinetic effects, at least in the first order, W_0 and τ_0 are linked with physical properties by two relations: $W_0 = d_0 \lambda / a_1$ and $\tau_0 = a_2 \lambda W_0^2 / D_l$, where $a_1 = 0.8839$ and $a_2 = 0.6267$ are numerical constants, λ is the coupling constant between the phase-field and concentration equations, $d_0 = \Gamma / (|m|c_0(1 - k)/k) = 0.013 \mu\text{m}$ is the capillary length. Simulations are carried out in two-dimensional systems with finite difference formulas on a fixed grid and time stepped with a simple Euler scheme. The grid size $\Delta x / W_0 = 0.4$ is used in all simulations. Periodic boundary conditions are imposed to reduce the domain size. The interface width is given by W_0 , and hence λ is seen as the numerical convergence parameter of this model.

A similar history results in a similar primary spacing in directional solidification of dendritic arrays [20,21]. Hence, a wide range of primary spacing can be selected in the same solidification condition. When the primary spacing is too low or too large, cell elimination or tertiary branching may occur. Within this finite range of primary spacing, adjustment of primary spacing Λ can be achieved by varying the initial wavelength of the interface. Therefore, the dynamical selection of primary spacing Λ in directional solidification is not addressed here. Unlike the experimental set-ups in Ref. [8–10], the direction of thermal gradient is parallel to the direction of pulling velocity, and hence $Pe = V_G \Lambda / D_l = V_p \Lambda / D_l$. Details of computational procedures can be found in Ref. [18]. Numerical simulations by Chen et al. [22] show that the dendrite-to-seaweed transition occurs once the artificial noise is sufficiently large. Three-dimensional phase-field simulations by Ghmadh et al. [12] show that results from numerical simulations with and without noise are in agreement with the DGP law. Our previous work

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